DISCRETE TOMOGRAPHY OF ICOSAHEDRAL MODEL SETS

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Abstract. The discrete tomography of B-type and F-type icosahedral model sets is investigated, with an emphasis on reconstruction and uniqueness problems. These are motivated by the request of materials science for the unique reconstruction of quasicrystalline structures from a small number of images produced by quantitative high resolution transmission electron microscopy.

1. Introduction

Discrete tomography (the word "tomography" is derived from the Greek $\tau o\mu o\sigma$, meaning a slice) is concerned with the inverse problem of retrieving information about some *finite* object from (generally noisy) information about its slices. A typical example is the *reconstruction* of a finite point set in Euclidean 3-space from its line sums in a small number of directions. More precisely, a (*discrete parallel*) *X-ray* of a finite subset of Euclidean d-space $\mathbb{R}^d$ in direction u gives the number of points of the set on each line in $\mathbb{R}^d$ parallel to u. This concept should not be confused with X-rays in diffraction theory, which provide rather different information on the underlying structure that is based on statistical pair correlations; compare [10], [12] and [19]. In the classical setting, motivated by crystals, the positions to be determined form a subset of a common translate of the cubic lattice $\mathbb{Z}^3$ or, more generally, of an arbitrary lattice L in $\mathbb{R}^3$. In fact, many of the problems in discrete tomography have been studied on $\mathbb{Z}^2$, the classical planar setting of discrete tomography; see [21], [17] and [16]. Beyond the case of perfect crystals, one has to take into account wider classes of sets, or at least significant deviations from the lattice structure. As an intermediate step between periodic and random (or amorphous) Delone sets, we consider systems of *aperiodic order*, more precisely, so-called *model sets* (or *mathematical quasicrystals*), which are commonly regarded as good mathematical models for quasicrystalline structures in nature [38].

Our interest in the discrete tomography of model sets is mainly motivated by the task of structure determination of quasicrystals, a new type of solids discovered 25 years ago; see [33] for the pioneering paper and [37, 25, 11] for background and applications. More precisely, we address the problem of uniquely reconstructing three-dimensional quasicrystals from their images under quantitative *high resolution transmission electron microscopy* (HRTEM) in a small number of directions. In fact, in [26] and [36] a technique is described, based on HRTEM, which can effectively measure the number of atoms lying on lines parallel to certain directions; it is called QUANTITEM (**QU**antitative **AN**alysis of **T**he **I**nformation from **T**ransmission **E**lectron **M**icroscopy). At present, the measurement of the number of atoms lying on a line can only be approximately achieved for some crystals; *cf.* [26, 36]. However, it is reasonable to expect that future developments in technology will improve this situation.

In this text, we consider both *B-type* and *F-type icosahedral model sets* $\varLambda$ in 3-space which can be described in algebraic terms by using the *icosian ring*; *cf.* [8], [27] and [29]. Note that the terminology originates from the fact that the underlying $\mathbb{Z}$-modules (to be explained in Section 3) of B-type and F-type icosahedral model sets can be obtained as projections of body-centred and face-centred hypercubic lattices in 6-space, respectively. The F-type icosahedral phase is the most common among the icosahedral quasicrystals. Below, we nevertheless develop the theory for both the B-type (also called I-type) and the F-type phase. Well known examples of icosahedral quasicrystals include the aluminium alloys AlMn and AlCuFe; *cf.* [22] for further examples.

In practice, only X-rays in $\varLambda$-directions, *i.e.*, directions parallel to non-zero elements of the difference set $\varLambda - \varLambda$ of $\varLambda$ (*i.e.*, the set of interpoint vectors of $\varLambda$) are reasonable. This is due to the fact that X-rays in non-$\varLambda$-directions are meaningless since the resolution coming from such X-rays would not be good enough to allow a quantitative analysis – neighbouring lines are not sufficiently separated. In fact, in order to obtain applicable results, one even has to find $\varLambda$-directions that guarantee HRTEM images of high resolution, *i.e.*, yield dense lines in the corresponding quasicrystal $\varLambda$.

Any lattice L in $\mathbb{R}^d$ can be sliced into lattices of dimension $d-1$. More generally, model sets have a dimensional hierarchy, *i.e.*, any model set in d dimensions can be sliced into model sets of dimension $d-1$. In Proposition 3.16, it is shown that *generic* (to be explained in Section 3) B-type and F-type icosahedral model sets can be sliced into (planar) *cyclotomic model sets*, whose discrete tomography we have studied earlier; *cf.* [4, 24] and [23]. The latter observation will be crucial, since it enables us to use the results on the discrete tomography of cyclotomic model sets, slice by slice.

Using the slicing of generic icosahedral model sets into cyclotomic model sets and the results from [4], it was shown in [24] that the algorithmic problem of *reconstructing* finite subsets of a large class of generic icosahedral model sets $\varLambda$ (*i.e.*, those with polyhedral windows) given X-rays in *two* $\varLambda$-directions can be solved in polynomial time in the real RAM-model of computation (Theorem 4.3). Since this *reconstruction problem* can possess rather different solutions, one is led to the investigation of the corresponding *uniqueness problem*, *i.e.*, the (unique) *determination* of finite subsets of a fixed icosahedral model set $\varLambda$ by X-rays in a small number of suitably prescribed $\varLambda$-directions. Here, a subset $\mathcal{E}$ of the set of all finite subsets of a fixed icosahedral model set $\varLambda$ is said to be *determined* by the X-rays in a finite set U of directions if different sets F and F' in $\mathcal{E}$ cannot have the same X-rays in the directions of U. Since, as demonstrated in Proposition 5.1, any fixed number of X-rays in $\varLambda$-directions is insufficient to determine the entire class of finite subsets of a fixed icosahedral model set $\varLambda$, it is necessary to impose some restriction in order to obtain positive uniqueness results. In Proposition 5.3, it is shown that the finite subsets F of cardinality less than or equal to some $k \in \mathbb{N}$ of a fixed icosahedral model set $\varLambda$ are determined by any set of $k+1$ X-rays in pairwise non-parallel $\varLambda$-directions. Proposition 5.6 then shows that, for every $R > 0$ and any fixed icosahedral model set $\varLambda$, there are two non-parallel $\varLambda$-directions such that the set of bounded subsets of $\varLambda$ with diameter less than R is determined by the X-rays in these directions. For our main result, we restrict the set of finite subsets of a fixed icosahedral model set $\varLambda$ by considering the class of *convex* subsets of $\varLambda$. They are finite sets $C \subset \varLambda$ whose convex hulls contain no new points of $\varLambda$, *i.e.*, finite sets $C \subset \varLambda$ with $C = \mathrm{conv}(C) \cap \varLambda$. By using the

slicing of generic icosahedral model sets into cyclotomic model sets again, it is shown that there are *four* pairwise non-parallel $\varLambda$-directions such that the set of convex subsets of any icosahedral model set $\varLambda$ are determined by their X-rays in these directions (Theorem 5.12). In fact, it turns out that one can choose four $\varLambda$-directions which provide uniqueness and yield dense lines in icosahedral model sets, the latter making this result look promising in view of real applications (Example 5.14 and Remark 5.15). Finally, we demonstrate that, in an approximative sense, this result holds in a far more general (and relevant) situation, where one deals with a whole family of generic icosahedral model sets at the same time, rather than dealing with a single fixed icosahedral model set.

2. Preliminaries and notation

Natural numbers are always assumed to be positive, *i.e.*, $\mathbb{N} = \{1, 2, 3, \dots\}$. Throughout the text, we use the convention that the symbol $\subset$ includes equality. We denote the norm in Euclidean d-space $\mathbb{R}^d$ by $\|\cdot\|$. The unit sphere in $\mathbb{R}^d$ is denoted by $\mathbb{S}^{d-1}$, *i.e.*, $\mathbb{S}^{d-1} = \{x \in \mathbb{R}^d \mid \|x\| = 1\}$. Moreover, the elements of $\mathbb{S}^{d-1}$ are also called *directions*. Recall that a *homothety* $h\colon \mathbb{R}^d \to \mathbb{R}^d$ is given by $x \mapsto \lambda x + t$, where $\lambda \in \mathbb{R}$ is positive and $t \in \mathbb{R}^d$. We call a homothety *expansive* if $\lambda > 1$. If $x \in \mathbb{R}$, then $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x. For $r > 0$ and $x \in \mathbb{R}^d$, $B_r(x)$ is the open ball of radius r about x. For a subset $S \subset \mathbb{R}^d$, $k \in \mathbb{N}$ and $R > 0$, we denote by $\operatorname{card}(S)$, $\mathcal{F}(S)$, $\mathcal{F}_{\leq k}(S)$, $\mathcal{D}_{<R}(S)$, $\operatorname{int}(S)$, $\operatorname{cl}(S)$, $\operatorname{bd}(S)$, $\operatorname{conv}(S)$, $\operatorname{diam}(S)$ and 1_S the cardinality, the set of finite subsets, the set of finite subsets of S having cardinality less than or equal to k, the set of subsets of S with diameter less than R, interior, closure, boundary, convex hull, diameter and characteristic function of S, respectively. The *centroid* (or *centre of mass*) of an element $F \in \mathcal{F}(\mathbb{R}^d)$ is defined as $(\sum_{f\in F} f)/\operatorname{card}(F)$. A linear subspace T of $\mathbb{R}^d$ is called an S-*subspace* if it is generated by elements of the *difference set* $S - S := \{s - s' \mid s, s' \in S\}$ of S. A direction $u \in \mathbb{S}^{d-1}$ is called an S-*direction* if it is parallel to a non-zero element of $S - S$. As usual, $R^\times$ denotes the group of units of a given ring R. Finally, for $(a, b, c)^t \in \mathbb{R}^3 \setminus \{0\}$, we denote by $H^{(a,b,c)}$ the hyperplane in $\mathbb{R}^3$ orthogonal to $(a, b, c)^t$.

Definition 2.1. Let $d \in \mathbb{N}$ and let $F \in \mathcal{F}(\mathbb{R}^d)$. Furthermore, let $u \in \mathbb{S}^{d-1}$ be a direction and let $\mathcal{L}_u^d$ be the set of lines in direction u in $\mathbb{R}^d$. Then, the (*discrete parallel*) *X-ray* of F *in direction* u is the function $X_uF : \mathcal{L}_u^d \to \mathbb{N}_0 := \mathbb{N} \cup \{0\}$, defined by

$$X_uF(\ell) := \operatorname{card}(F \cap \ell\,) = \sum_{x\in\ell} 1_F(x)\,.$$

Moreover, the *support* $(X_uF)^{-1}(\mathbb{N})$ of X_uF, *i.e.*, the set of lines in $\mathcal{L}_u^d$ which pass through at least one point of F, is denoted by $\operatorname{supp}(X_uF)$. For $z \in \mathbb{R}^d$, we denote by ℓ_u^z the element of $\mathcal{L}_u^d$ which passes through z. Moreover, for $S \subset \mathbb{R}^d$, we denote by $\mathcal{L}_u^S$ the subset of $\mathcal{L}_u^d$ consisting of all elements of the form ℓ_u^z, where $z \in S$, *i.e.*, lines in $\mathcal{L}_u^d$ which pass through at least one point of S.

Lemma 2.2. [14, Lemma 5.1 and Lemma 5.4] *Let $d \in \mathbb{N}$ and let $u \in \mathbb{S}^{d-1}$ be a direction. For all $F, F' \in \mathcal{F}(\mathbb{R}^d)$, one has:*

(a) $X_uF = X_uF'$ *implies* $\operatorname{card}(F) = \operatorname{card}(F')$.
(b) *If $X_uF = X_uF'$, the centroids of F and F' lie on the same line parallel to u.*

Definition 2.3. Let $d \geq 2$, let $U \subset \mathbb{S}^{d-1}$ be a finite set of pairwise non-parallel directions and let $F \in \mathcal{F}(\mathbb{R}^d)$. We define the *grid* of F with respect to the X-rays in the directions of U as

$$G_U^F := \bigcap_{u\in U} \left(\bigcup_{\ell \in \operatorname{supp}(X_u F)} \ell \right).$$

The following property follows immediately from the definition of grids.

Lemma 2.4. *Let $d \geq 2$. If $U \subset \mathbb{S}^{d-1}$ is a finite set of pairwise non-parallel directions, then for all $F, F' \in \mathcal{F}(\mathbb{R}^d)$, one has*

$$(X_u F = X_u F' \;\forall u \in U) \implies F, F' \subset G_U^F = G_U^{F'}.$$

Definition 2.5. Let $d \geq 2$, let $\mathcal{E} \subset \mathcal{F}(\mathbb{R}^d)$, and let $m \in \mathbb{N}$. Further, let $U \subset \mathbb{S}^{d-1}$ be a finite set of directions. We say that $\mathcal{E}$ is *determined* by the X-rays in the directions of U if, for all $F, F' \in \mathcal{E}$, one has

$$(X_u F = X_u F' \;\forall u \in U) \implies F = F'.$$

Further, we say that $\mathcal{E}$ is *determined* by m X-rays if there exists a set U of m pairwise non-parallel directions such that $\mathcal{E}$ is determined by the X-rays in the directions of U.

The following property is straight-forward.

Lemma 2.6. *Let $d \geq 2$, let $h\colon \mathbb{R}^d \to \mathbb{R}^d$ be a homothety, and let $U \subset \mathbb{S}^{d-1}$ be a finite set of directions. Then, if F and F' are elements of $\mathcal{F}(\mathbb{R}^d)$ with the same X-rays in the directions of U, the images $h(F)$ and $h(F')$ also have the same X-rays in the directions of U.*

Gardner and Gritzmann introduced the so-called *convex lattice sets*, *i.e.*, finite subsets C of some lattice $L \subset \mathbb{R}^d$ with $C = \operatorname{conv}(C) \cap L$; *cf.* [14, Section 2]. More generally, we define as follows.

Definition 2.7. Let $d \in \mathbb{N}$ and let $S \subset \mathbb{R}^d$. A finite subset C of S is called a *convex subset of S* if it satisfies the equation $C = \operatorname{conv}(C) \cap S$. Moreover, the set of all convex subsets of S is denoted by $\mathcal{C}(S)$.

3. Icosahedral model sets

We shall always denote the golden ratio by τ, *i.e.*, $\tau = (1+\sqrt{5})/2$. Moreover, by $.'$ we will denote the unique non-trivial Galois automorphism of the real quadratic number field $\mathbb{Q}(\tau) = \mathbb{Q}(\sqrt{5}) = \mathbb{Q} \oplus \mathbb{Q}\tau$ (determined by $\sqrt{5} \mapsto -\sqrt{5}$), whence $\tau' = -1/\tau = 1 - \tau$. Note that τ is an algebraic integer (a root of $X^2 - X - 1 \in \mathbb{Z}[X]$) of degree 2 over $\mathbb{Q}$. Moreover, $\mathbb{Z}[\tau] = \mathbb{Z} \oplus \mathbb{Z}\tau$ is the ring of integers in $\mathbb{Q}(\tau)$ and, for its group of units, one further has $\mathbb{Z}[\tau]^\times = \{\tau^s \mid s \in \mathbb{Z}\}$ (*i.e.*, τ is a fundamental unit of $\mathbb{Z}[\tau]$); *cf.* [20].

3.1. Definition and properties of icosahedral model sets.

Let $\mathbb{H}$ be the skew field of *Hamiltonian quaternions*, *i.e.*,

$$\mathbb{H} = \{a + bi + cj + dk \mid a, b, c, d \in \mathbb{R}\},$$

a four-dimensional vector space over $\mathbb{R}$ with a non-commutative multiplication determined by the following relations for the generating elements 1 (implicit in the above representation) and i, j, k:

$$i^2 = j^2 = k^2 = ijk = -1,$$

together with the requirement that $\mathbb{R}$ is central in $\mathbb{H}$. Note that $\mathbb{R}$ is precisely the center of $\mathbb{H}$. The *conjugate* of $\alpha = a + bi + cj + dk \in \mathbb{H}$ is defined by $\bar{\alpha} = a - bi - cj - dk$, the *reduced norm* by $\mathrm{nr}(\alpha) = \alpha\bar{\alpha} = a^2 + b^2 + c^2 + d^2$ and the *reduced trace* by $\mathrm{tr}(\alpha) = \alpha + \bar{\alpha} = 2a$. Moreover, we shall sometimes call $\mathrm{Re}(\alpha) := a \in \mathbb{R}$ the *real part* and $\mathrm{Im}(\alpha) := (b, c, d)^t \in \mathbb{R}^3$ the *imaginary part* of α. Let $\mathbb{H}_0$ be the set of quaternions with real part 0, *i.e.*,

$$\mathbb{H}_0 := \{\alpha \in \mathbb{H} \mid \mathrm{tr}(\alpha) = 0\} = \{bi + cj + dk \mid b, c, d \in \mathbb{R}\} \;\simeq\; \mathbb{R}^3 .$$

The *icosian ring* $\mathbb{I}$ (*cf.* [8, 27, 29]) is the additive subgroup of $\mathbb{H}$ that is given by the integer linear combinations of the quaternions

$$\big((\pm 1, 0, 0, 0)^t\big)^{\mathsf{A}}, \tfrac{1}{2}\left((\pm 1, \pm 1, \pm 1, \pm 1)^t\right)^{\mathsf{A}}, \tfrac{1}{2}\left((0, \pm 1, \pm\tau', \tau)^t\right)^{\mathsf{A}} ,$$

where we identify $\mathbb{H}$ with $\mathbb{R}^4$ via the basis $\{1, i, j, k\}$ and, as in [9, Chapter 8], the superscript A indicates that all even permutations of the coordinates are allowed. The members of $\mathbb{I}$ are called *icosians*. Note that $\mathbb{I}$ is a ring, because these generators (which have reduced norm 1) form a multiplicative group, the *icosian group*, of order 120. Note further that $\mathbb{I}$ is also a free $\mathbb{Z}[\tau]$-module of rank 4. By [7], $\mathbb{I}$ is a maximal order of the quaternion algebra $\mathbb{H}(\mathbb{Q}(\tau))$ over $\mathbb{Q}(\tau)$, defined similar to $\mathbb{H}$ as

$$\mathbb{H}\big(\mathbb{Q}(\tau)\big) = \big\{a + bi + cj + dk \,\big|\, a, b, c, d \in \mathbb{Q}(\tau)\big\} .$$

The set

$$\mathbb{I}_0 \;:=\; \mathrm{Im}(\mathbb{I} \cap \mathbb{H}_0) \;\subset\; \mathbb{R}^3$$

of 'pure imaginary' icosians is generated as an additive group by the elements

$$\big((\pm 1, 0, 0)^t\big)^{\mathsf{A}}, \tfrac{1}{2}\left((\pm 1, \pm\tau', \pm\tau)^t\right)^{\mathsf{A}} ,$$

where the superscript A is defined as above. Consider the standard body-centred icosahedral module $\mathcal{M}_{\mathrm{B}}$ of quasicrystallography, defined as

$$\begin{aligned}
\mathcal{M}_{\mathrm{B}} \;&:=\; \mathbb{Z}[\tau](2,0,0)^t \oplus \mathbb{Z}[\tau](1,1,1)^t \oplus \mathbb{Z}[\tau](\tau,0,1)^t \\
&=\; \mathbb{Z}[\tau](0,2,0)^t \oplus \mathbb{Z}[\tau](-1,-\tau',\tau)^t \oplus \mathbb{Z}[\tau](1,1,1)^t \\
&=\; \left\{ (\beta,\gamma,\delta)^t \;\middle|\; \begin{array}{l} \beta,\gamma,\delta \in \mathbb{Z}[\tau], \text{ with} \\ \tau^2\beta + \tau\gamma + \delta \equiv\; 0 \;(\mathrm{mod}\, 2) \end{array} \right\} ;
\end{aligned} \tag{1}$$

cf. [2, 7] and references therein. One has $\mathrm{Im}(\mathbb{I}) = \frac{1}{2}\mathcal{M}_{\mathrm{B}}$ and, further, $\mathbb{I}_0 = \frac{1}{2}\mathcal{M}_{\mathrm{F}}$, where $\mathcal{M}_{\mathrm{F}}$ is the standard face-centred icosahedral module of quasicrystallography, defined as

$$\begin{aligned}
\mathcal{M}_{\mathrm{F}} \;&:=\; \left\{ (\beta,\gamma,\delta)^t \;\middle|\; \begin{array}{l} \beta,\gamma,\delta \in \mathbb{Z}[\tau], \text{ with} \\ \beta \equiv \tau\gamma \equiv \tau^2\delta \;(\mathrm{mod}\, 2) \end{array} \right\} \\
&=\; \big\{ (\beta,\gamma,\delta)^t \in \mathcal{M}_{\mathrm{B}} \,\big|\, \beta + \gamma + \delta \equiv\; 0 \;(\mathrm{mod}\, 2) \big\} \\
&=\; \mathbb{Z}[\tau](2,0,0)^t \oplus \mathbb{Z}[\tau](\tau+1,\tau,1)^t \oplus \mathbb{Z}[\tau](0,0,2)^t \\
&=\; \mathbb{Z}[\tau](0,2,0)^t \oplus \mathbb{Z}[\tau](-1,-\tau',\tau)^t \oplus \mathbb{Z}[\tau](2,0,0)^t \;\overset{4}{\subset}\; \mathcal{M}_{\mathrm{B}} ,
\end{aligned} \tag{2}$$

where integers on top of the inclusion symbol denote the corresponding subgroup indices; *cf.* [2, 7] again. Both $\mathcal{M}_{\mathrm{B}}$ and $\mathcal{M}_{\mathrm{F}}$ are free $\mathbb{Z}[\tau]$-modules of rank 3, and are hence $\mathbb{Z}$-modules of rank 6. Moreover, both $\mathcal{M}_{\mathrm{B}}$ and $\mathcal{M}_{\mathrm{F}}$ have icosahedral symmetry, *i.e.*, they are invariant

under the action of the rotation group Y. This group is generated by the rotations which are given, with respect to the canonical basis, by the following matrices

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix} \tau & -1 & -\tau' \\ 1 & -\tau' & -\tau \\ -\tau' & \tau & 1 \end{pmatrix}. \tag{3}$$

Note that Y is the rotation group of the regular icosahedron centred at the origin $0 \in \mathbb{R}^3$ with orientation such that each coordinate axis passes through the mid-point of an edge, thus coinciding with 2-fold axes of the icosahedron. Moreover, the matrix on the left (resp., on the right) is an order 2 (resp., order 5) rotation.

Remark 3.1. There is another $\mathbb{Z}$-module of rank 6, intermediate between $\mathcal{M}_{\mathrm{F}}$ and $\mathcal{M}_{\mathrm{B}}$, which also has icosahedral symmetry. This is the standard primitive icosahedral module $\mathcal{M}_{\mathrm{P}}$, defined as

$$\mathcal{M}_{\mathrm{P}} \;:=\; \left\{ (\beta,\gamma,\delta)^t \in \mathcal{M}_{\mathrm{B}} \,\middle|\, \beta+\gamma+\delta \equiv\; 0 \text{ or } \tau \pmod 2 \right\}.$$

In contrast to $\mathcal{M}_{\mathrm{F}}$ and $\mathcal{M}_{\mathrm{B}}$, $\mathcal{M}_{\mathrm{P}}$ fails to be a $\mathbb{Z}[\tau]$-module. In fact, $\mathcal{M}_{\mathrm{P}}$ is a $\mathbb{Z}[2\tau]$-module only, and it is a $\mathbb{Z}$-module of rank 6.

By definition, *model sets* arise from so-called *cut and project schemes*; *cf.* [6, 27] for general background material and see [3] for a gentle introduction. In the case of Euclidean internal spaces, these are commutative diagrams of the following form, where π and π_{int} denote the canonical projections; *cf.* [27].

$$\begin{array}{ccccc} \mathbb{R}^d & \stackrel{\pi}{\longleftarrow} & \mathbb{R}^d \times \mathbb{R}^m & \stackrel{\pi_{\mathrm{int}}}{\longrightarrow} & \mathbb{R}^m \\ \cup & & \cup \text{ lattice} & & \cup \text{ dense} \\ L & \stackrel{1\text{–}1}{\longleftrightarrow} & \widetilde{L} & \longrightarrow & L^\star \end{array} \tag{4}$$

Here, $\tilde{L}$ is a lattice in $\mathbb{R}^d \times \mathbb{R}^m$. Further, we assume that the restriction $\pi|_{\tilde{L}}$ is injective and that the image $\pi_{\mathrm{int}}(\tilde{L})$ is a dense subset of $\mathbb{R}^m$. Letting $L := \pi(\tilde{L})$, the bijectivity of the (co-)restriction $\pi|_{\tilde{L}}^{L}$ allows us to define a map $.^\star\colon\, L \to \mathbb{R}^m$ by $\alpha^\star := \pi_{\mathrm{int}}((\pi|_{\tilde{L}}^{L})^{-1}(\alpha))$. Then, one has $L^\star = \pi_{\mathrm{int}}(\tilde{L})$ and, further, $\tilde{L} = \{(l, l^\star) \,|\, l \in L\}$.

Definition 3.2. Given a subset $W \subset \mathbb{R}^m$ with $\varnothing \neq \mathrm{int}(W) \subset W \subset \mathrm{cl}(\mathrm{int}(W))$ and $\mathrm{cl}(\mathrm{int}(W))$ compact, a so-called *window*, and any $t \in \mathbb{R}^d$, we obtain a model set

$$\varLambda(t, W) := t + \varLambda(W)$$

relative to the above cut and project scheme (4) by setting

$$\varLambda(W) := \{\alpha \in L \,|\, \alpha^\star \in W\}.$$

Moreover, $\mathbb{R}^d$ (resp., $\mathbb{R}^m$) is called the *physical* (resp., *internal*) space. The map $.^\star\colon\, L \to \mathbb{R}^m$, as defined above, is the so-called *star map* of $\varLambda(t, W)$, W is referred to as the *window* of $\varLambda(t, W)$ and L is the so-called *underlying* $\mathbb{Z}$*-module of* $\varLambda(t, W)$. The model set $\varLambda(t, W)$ is called *generic* if it satisfies $\mathrm{bd}(W) \cap L^\star = \varnothing$. Moreover, it is called *regular* if the boundary $\mathrm{bd}(W)$ has Lebesgue measure 0 in $\mathbb{R}^m$.

Remark 3.3. Every translate of a window $W \subset \mathbb{R}^m$ is a window again.

Definition 3.4. *B-type icosahedral model sets* $\varLambda^{\mathrm{B}}_{\mathrm{ico}}(t, W)$ arise from the cut and project scheme (4) by setting $d := m := 3$, $L := \mathrm{Im}(\mathbb{I})$ and letting the star map $.^\star\colon \mathrm{Im}(\mathbb{I}) \to \mathbb{R}^3$ be defined by applying the Galois conjugation $.'$ to each coordinate of an element $\alpha \in \mathrm{Im}(\mathbb{I})$. We denote by $\mathcal{I}^{\mathrm{B}}$ the set of all B-type icosahedral model sets and define $\mathcal{I}^{\mathrm{B}}_g$ as the subset of all generic B-type icosahedral model sets. Additionally, for a window $W \subset \mathbb{R}^3$, we set

$$\mathcal{I}^{\mathrm{B}}_g(W) \;:=\; \{\varLambda^{\mathrm{B}}_{\mathrm{ico}}(t, s+W) \,|\, t, s \in \mathbb{R}^3\} \;\cap\; \mathcal{I}^{\mathrm{B}}_g\,.$$

F-type icosahedral model sets $\varLambda^{\mathrm{F}}_{\mathrm{ico}}(t, W)$ arise from the cut and project scheme (4) by setting $d := m := 3$, $L := \mathbb{I}_0$ and letting the star map $.^\star\colon \mathbb{I}_0 \to \mathbb{R}^3$ again be defined by applying the Galois conjugation $.'$ to each coordinate of an element $\alpha \in \mathbb{I}_0$. Moreover, the sets $\mathcal{I}^{\mathrm{F}}$, $\mathcal{I}^{\mathrm{F}}_g$ and $\mathcal{I}^{\mathrm{F}}_g(W)$, where $W \subset \mathbb{R}^3$ is a window, are defined similarly. Below, we say that $\varLambda_{\mathrm{ico}}(t, W)$ is an *icosahedral model set* if $\varLambda_{\mathrm{ico}}(t, W) = \varLambda^{\mathrm{B}}_{\mathrm{ico}}(t, W)$ or $\varLambda_{\mathrm{ico}}(t, W) = \varLambda^{\mathrm{F}}_{\mathrm{ico}}(t, W)$. Finally, B-type (resp., F-type) icosahedral model sets are also referred to as *icosahedral model sets with underlying* $\mathbb{Z}$*-module* $\mathrm{Im}(\mathbb{I})$ (resp., $\mathbb{I}_0$).

Remark 3.5. Both star maps as defined in Definition 3.4 are $\mathbb{Q}$-linear monomorphism of Abelian groups and naturally extend to a monomorphism $\mathbb{Q}(\tau)^3 \to \mathbb{R}^3$, which we also denote by $.^\star$. Both in the B-type and the F-type case, we shall denote by $.^{-\star}$ the inverse of the co-restriction of the corresponding star map $.^\star\colon L \to L^\star$ to its image. The images of both maps $\widetilde{.}\colon L \to \mathbb{R}^3 \times \mathbb{R}^3$, defined by $\alpha \mapsto (\alpha, \alpha^\star)$, are indeed lattices in $\mathbb{R}^3 \times \mathbb{R}^3 \simeq \mathbb{R}^6$. In fact, these images have a natural interpretation as a weight lattice of type D_6^* in the B-type case and a root lattice of type D_6 in the F-type case; *cf.* [8, 9] for background. Finally, one can easily verify that the images $\mathrm{Im}(\mathbb{I})^\star$ and $\mathbb{I}_0{}^\star$ are indeed dense subsets of $\mathbb{R}^3$.

We refer the reader to [27, 30] for details and related general settings, and to [6] for general background. Before we collect some properties of icosahedral model sets, recall the following notions. A subset $\varLambda$ of $\mathbb{R}^d$ is called *uniformly discrete* if there is a radius $r > 0$ such that every ball $B_r(x)$ with $x \in \mathbb{R}^d$ contains at most one point of $\varLambda$. Further, $\varLambda$ is called *relatively dense* if there is a radius $R > 0$ such that every ball $B_R(x)$ with $x \in \mathbb{R}^d$ contains at least one point of $\varLambda$.

Remark 3.6. Let $\varLambda$ be an icosahedral model set with window W. Then, $\varLambda$ is a *Delone set* in $\mathbb{R}^3$ (*i.e.*, $\varLambda$ is both uniformly discrete and relatively dense) and is of *finite local complexity* (*i.e.*, $\varLambda - \varLambda$ is closed and discrete). Note that $\varLambda$ is of finite local complexity if and only if for every $r > 0$ there are, up to translation, only finitely many point sets (called *patches of diameter* r) of the form $\varLambda \cap B_r(x)$, where $x \in \mathbb{R}^3$; *cf.* [35, Proposition 2.3]. In fact, $\varLambda$ is even a *Meyer set*, *i.e.*, $\varLambda$ is a Delone set and $\varLambda - \varLambda$ is uniformly discrete; compare [27]. Further, $\varLambda$ is an *aperiodic* model set, *i.e.*, $\varLambda$ has no translational symmetries. Moreover, if $\varLambda$ is *regular*, $\varLambda$ is *pure point diffractive*, *i.e.*, the Fourier transform of the autocorrelation density that arises by placing a delta peak (point mass) on each point of $\varLambda$ looks purely point-like; *cf.* [35]. If $\varLambda$ is generic, $\varLambda$ is *repetitive*, *i.e.*, given any patch of radius r, there is a radius $R > 0$ such that any ball of radius R contains at least one translate of this patch; *cf.* [35]. If $\varLambda$ is regular, the frequency of repetition of finite patches is well defined, *i.e.*, for any patch of radius r, the number of occurrences of translates of this patch per unit volume in the ball $B_r(0)$ of radius $r > 0$ about the origin 0 approaches a non-negative limit as $r \to \infty$; *cf.* [34]. Moreover, if $\varLambda$ is both generic

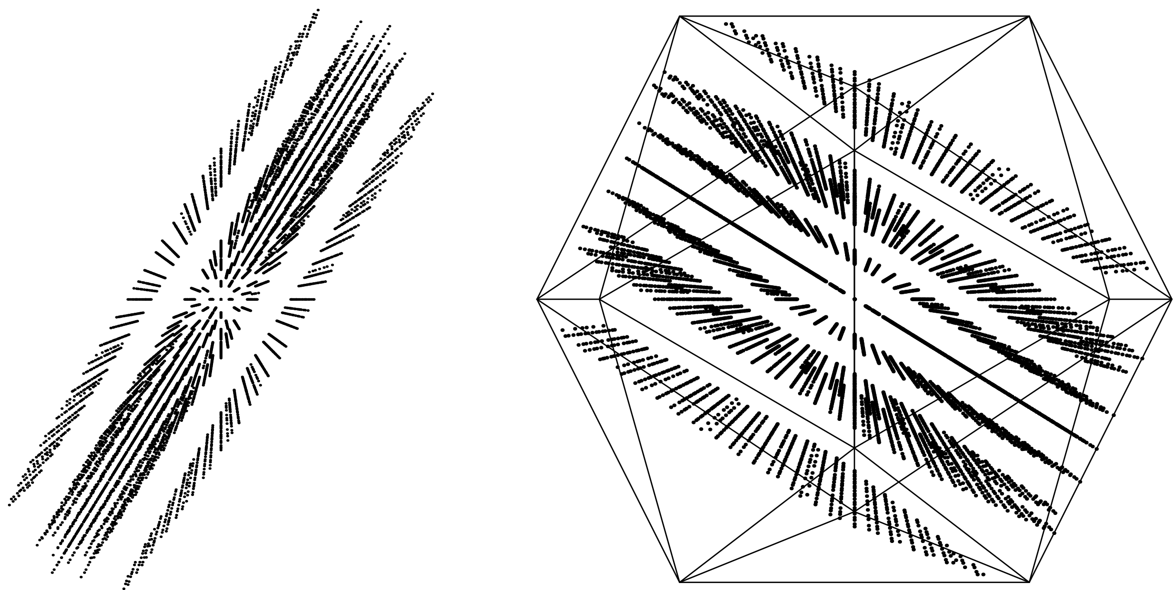

FIGURE 1. A few slices of a patch of the icosahedral model set $\varLambda_{\text{ico}}^{\text{B}}$ (left) and their $.^{\star}$-images inside the icosahedral window in the internal space (right), both seen from the positive x-axis.

and regular, and, if a suitable translate of the window W has full icosahedral symmetry (*i.e.*, if a suitable translate of the window W is invariant under the action of the group $Y_h^{\star}$ of order 120, where $Y_h^{\star} := Y^{\star} \cup (-Y^{\star})$ and $Y^{\star}$ is the group of rotations of order 60 generated by the two matrices that arise from the two matrices in (3) by applying the conjugation $.'$ to each entry), then $\varLambda$ has full icosahedral symmetry $Y_h := Y \cup (-Y)$ in the sense of symmetries of LI-classes, meaning that a discrete structure has a certain symmetry if the original and the transformed structure are locally indistinguishable (LI) (*i.e.*, up to translation, every *finite* patch in $\varLambda$ also appears in any of the other elements of its LI-class and *vice versa*); see [3] for details. Typical examples are balls and suitably oriented versions of the icosahedron, the dodecahedron, the rhombic triacontahedron (the latter also known as Kepler's body) and its dual, the icosidodecahedron.

Example 3.7. For a generic regular icosahedral model set with full icosahedral symmetry Y_h, consider $\varLambda_{\text{ico}}^{\text{B}} := \varLambda_{\text{ico}}^{\text{B}}(0, s + W)$, where $s := 10^{-3}(1,1,1)^t$ and W is the regular icosahedron with vertex set $Y_h^{\star}(\tau', 0, 1)^t$; see Figure 1 for an illustration.

3.2. **Cyclotomic model sets as planar sections of icosahedral model sets.** In this section, we shall demonstrate that both B-type and F-type icosahedral model sets $\varLambda$ can be nicely sliced into *cyclotomic model sets with underlying* $\mathbb{Z}$*-module* $\mathbb{Z}[\zeta_5]$, where the slices are intersections of $\varLambda$ with translates of the hyperplane $H^{(\tau,0,1)}$ in $\mathbb{R}^3$ orthogonal to $(\tau, 0, 1)^t$.

From now on, we always let $\zeta_5 := e^{2\pi i/5}$, as a specific choice of a primitive 5th root of unity in $\mathbb{C}$. Occasionally, we identify $\mathbb{C}$ with $\mathbb{R}^2$.

Remark 3.8. It is well known that the 5th cyclotomic field $\mathbb{Q}(\zeta_5)$ is an algebraic number field of degree 4 over $\mathbb{Q}$. Moreover, the field extension $\mathbb{Q}(\zeta_5)/\mathbb{Q}$ is a Galois extension with Abelian Galois group $G(\mathbb{Q}(\zeta_5)/\mathbb{Q}) \simeq (\mathbb{Z}/5\mathbb{Z})^\times$, where $a \,(\mathrm{mod}\, 5)$ corresponds to the automorphism given by $\zeta_5 \mapsto \zeta_5^a$; *cf.* [39, Theorem 2.5]. Note that, restricted to the quadratic field $\mathbb{Q}(\tau)$, both the Galois automorphism of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$ that is given by $\zeta_5 \mapsto \zeta_5^3$ and its complex conjugate automorphism (*i.e.*, the automorphism given by $\zeta_5 \mapsto \zeta_5^2$) induce the unique non-trivial Galois automorphism $.'$ of $\mathbb{Q}(\tau)/\mathbb{Q}$ (determined by $\tau \mapsto 1-\tau$). Further, $\mathbb{Z}[\zeta_5]$ is the ring of integers in $\mathbb{Q}(\zeta_5)$; *cf.* [39, Theorem 2.6]. The ring $\mathbb{Z}[\zeta_5]$ also is a $\mathbb{Z}[\tau]$-module of rank two. More precisely, one has the equality $\mathbb{Z}[\zeta_5] = \mathbb{Z}[\tau] \oplus \mathbb{Z}[\tau]\zeta_5$; *cf.* [4, Lemma 1(a)]. Since ζ_5^3 is also a primitive 5th root of unity in $\mathbb{C}$, one further has the equality $\mathbb{Z}[\zeta_5] = \mathbb{Z}[\zeta_5^3] = \mathbb{Z}[\tau] \oplus \mathbb{Z}[\tau]\zeta_5^3$.

Definition 3.9. *Cyclotomic model sets with underlying* $\mathbb{Z}$*-module* $\mathbb{Z}[\zeta_5]$ $\varLambda_{\mathrm{cyc}}(t, W)$ arise from the cut and project scheme (4) by setting $d := m := 2$, $L := \mathbb{Z}[\zeta_5]$ and letting the star map $.^{\star_5}\colon L \to \mathbb{R}^2$ be either given by the non-trivial Galois automorphism of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$, defined by $\zeta_5 \mapsto \zeta_5^3$, or its complex conjugate automorphism.

Remark 3.10. The star map $.^{\star_5}$ as defined in Definition 3.9 is a monomorphism of Abelian groups. Further, the image of the map $\tilde{.}^{5}\colon L \to \mathbb{R}^2 \times \mathbb{R}^2$, defined by $\alpha \mapsto (\alpha, \alpha^{\star_5})$, is indeed a lattice in $\mathbb{R}^2 \times \mathbb{R}^2$. Finally, one can verify that the image $L^{\star_5}$ is indeed a dense subset of $\mathbb{R}^2$. For the general setting, we refer the reader to [4, 24, 23]. By [24, Lemma 1.84(a)] (see also [23, Lemma 25(a)]), for all cyclotomic model sets $\varLambda$ with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$, the set of $\varLambda$-directions is precisely the set of $\mathbb{Z}[\zeta_5]$-directions.

Example 3.11. For illustrations of cyclotomic model sets with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$, see Figure 2 on the left and Figure 3; *cf.* Proposition 3.16 and Example 3.17 below.

Lemma 3.12. *For* $L \in \{\mathrm{Im}(\mathbb{I}), \mathbb{I}_0\}$*, the following equations hold:*

(a) $L \cap H^{(\tau,0,1)} = \mathbb{Z}[\tau](0,1,0)^t \oplus \mathbb{Z}[\tau]\frac{1}{2}(-1,-\tau',\tau)^t$.

(b) $(L \cap H^{(\tau,0,1)})^\star = L^\star \;\cap\; H^{(\tau',0,1)}$.

Proof. Part (a) follows from Equations (1) and (2) together with the relations $\mathrm{Im}(\mathbb{I}) = \frac{1}{2}\mathcal{M}_{\mathrm{B}}$ and $\mathbb{I}_0 = \frac{1}{2}\mathcal{M}_{\mathrm{F}}$. Part (b) follows from the identity $((\tau,0,1)^t)^\star = (\tau',0,1)^t$. □

Definition 3.13. We denote by Φ the $\mathbb{R}$-linear isomorphism $\Phi\colon\ H^{(\tau,0,1)} \to \mathbb{C}$, determined by $(0,1,0)^t \mapsto 1$ and $\frac{1}{2}(-1,-\tau',\tau)^t \mapsto \zeta_5$. Further, $\Phi^\star$ will denote the $\mathbb{R}$-linear isomorphism $\Phi^\star\colon\ H^{(\tau',0,1)} \to \mathbb{C}$, determined by $(0,1,0)^t \mapsto 1$ and $\frac{1}{2}(-1,-\tau,\tau')^t \mapsto \zeta_5^3$.

Lemma 3.14. *The maps* Φ *and* $\Phi^\star$ *are isometries of Euclidean vector spaces, where* $H^{(\tau,0,1)}$*,* $H^{(\tau',0,1)}$ *and* $\mathbb{C}$ *are regarded as two-dimensional Euclidean vector spaces in the canonical way. Moreover, identifying* $\mathbb{C}$ *with the xy-plane in* $\mathbb{R}^3$*,* Φ *and* $\Phi^\star$ *extend uniquely to direct rigid motions of* $\mathbb{R}^3$*, i.e., elements of the group* $\mathrm{SO}(3,\mathbb{R})$*.*

Proof. The first assertion follows from the following identities:

$$\big\| r(0,1,0)^t + s\tfrac{1}{2}(-1,-\tau',\tau)^t \big\| = |r + s\,\zeta_5| = \sqrt{r^2+s^2-rs\tau'}\,,$$
$$\big\| r(0,1,0)^t + s\tfrac{1}{2}(-1,-\tau,\tau')^t \big\| = |r + s\,\zeta_5^3| = \sqrt{r^2+s^2-rs\tau}\,.$$

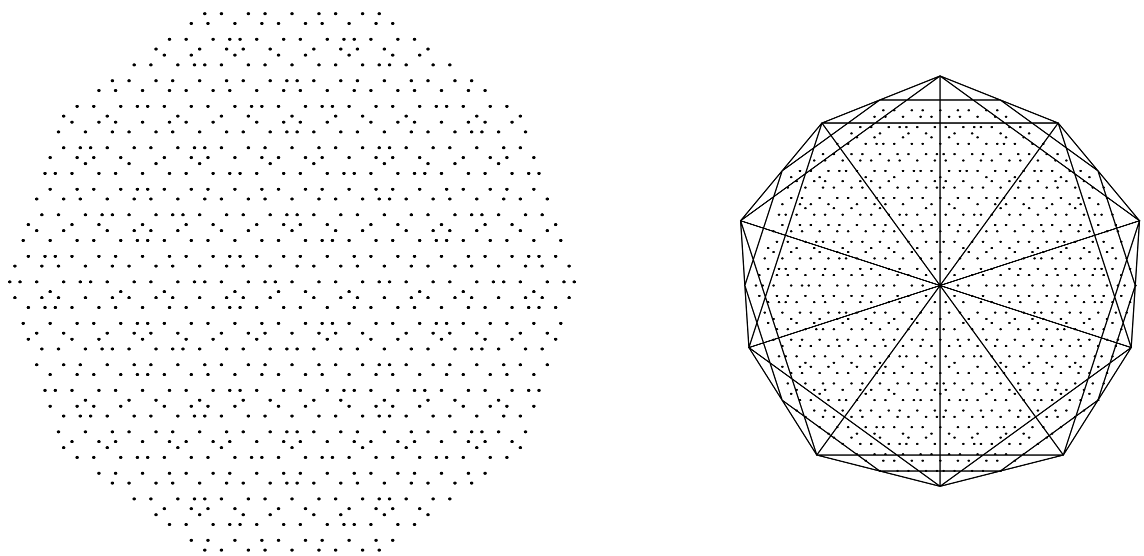

FIGURE 2. The central slice of the patch of $\varLambda_{\mathrm{ico}}^{\mathrm{B}}$ from Figure 1 (left) and its $.^{\star}$-image inside the (marked) decagon $(s+W)\cap H^{(\tau',0,1)}$ (right), both seen from perpendicular viewpoints.

The additional statement is immediate. □

Lemma 3.15. *Let $L\in\{\mathrm{Im}(\mathbb{I}),\mathbb{I}_0\}$. Via restriction, the maps Φ and $\Phi^{\star}$ induce isomorphisms of rank two $\mathbb{Z}[\tau]$-modules:*

$$L\cap H^{(\tau,0,1)}\xrightarrow{\Phi}\mathbb{Z}[\zeta_5]\,,$$
$$L^{\star}\cap H^{(\tau',0,1)}\xrightarrow{\Phi^{\star}}\mathbb{Z}[\zeta_5]\,.$$

Proof. This follows immediately from the definition of Φ and $\Phi^{\star}$ together with Lemma 3.12 and Remark 3.8. □

Proposition 3.16. *Let $\varLambda$ be a generic icosahedral model set with underlying $\mathbb{Z}$-module L, say $\varLambda=\varLambda_{\mathrm{ico}}(t,W)$. Then, for every $\lambda\in\varLambda$, one has the identity*

$$\Phi\big((\varLambda\ \cap\ (\lambda+H^{(\tau,0,1)}))-\lambda\big)\ =\ \big\{z\in\mathbb{Z}[\zeta_5]\,\big|\,z^{\star_5}\in W_{\lambda}\big\}\,,$$

where $.^{\star_5}$ is the Galois automorphism of $\mathbb{Q}(\zeta_5)/\mathbb{Q}$, defined by $\zeta_5\mapsto\zeta_5^3$ and

$$W_{\lambda}:=\Phi^{\star}\big((W\ \cap\ ((\lambda-t)^{\star}+H^{(\tau',0,1)}))-(\lambda-t)^{\star}\big)\,.$$

Thus, the sets of the form

$$\Phi\big((\varLambda\ \cap\ (\lambda+H^{(\tau,0,1)}))-\lambda\big)\,, \tag{5}$$

where $\lambda\in\varLambda$, are cyclotomic model sets with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$.

Proof. First, consider $\Phi(\mu)$, where $\mu\in(\varLambda\cap(\lambda+H^{(\tau,0,1)}))-\lambda$. It follows that $\mu\in L\cap H^{(\tau,0,1)}$ and $(\mu+(\lambda-t))^{\star}=\mu^{\star}+(\lambda-t)^{\star}\in W$. Lemma 3.15 implies that $\Phi(\mu)\in\mathbb{Z}[\zeta_5]$, say $\Phi(\mu)=\alpha+\beta\zeta_5$ for suitable $\alpha,\beta\in\mathbb{Z}[\tau]$. One has

$$\Phi(\mu)^{\star_5}\ =\ \alpha'+\beta'\zeta_5^3\ =\ \Phi^{\star}(\mu^{\star})\ \in\ W_{\lambda}\,.$$

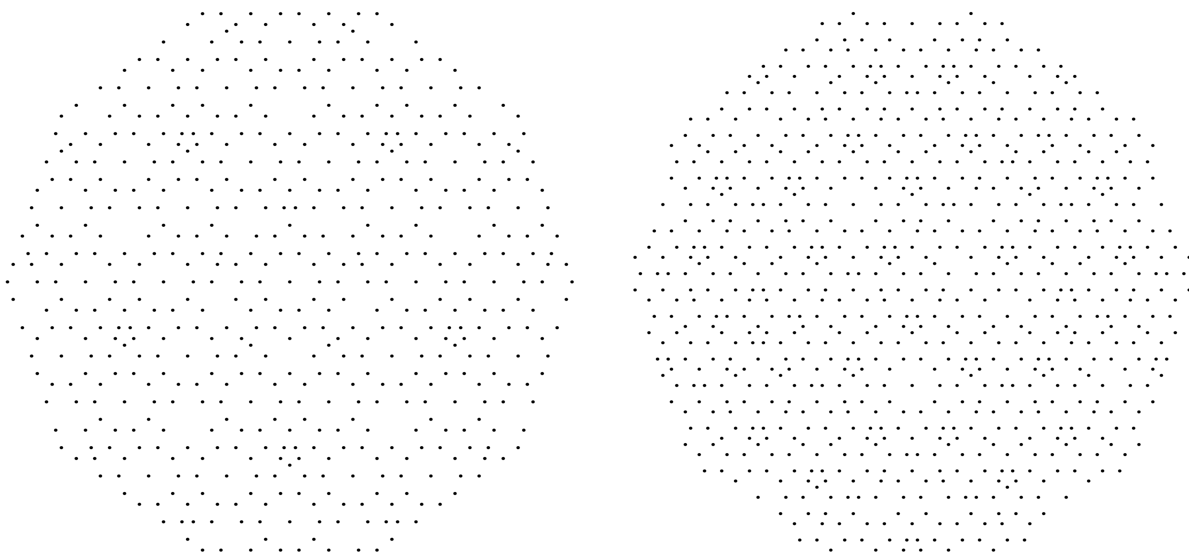

FIGURE 3. Another two slices of the patch of $\varLambda_{\mathrm{ico}}^{\mathrm{B}}$ from Figure 1.

Conversely, suppose that $z \in \mathbb{Z}[\zeta_5]$ satisfies $z^{\star_5} \in W_\lambda$. Then, there are suitable $\alpha, \beta \in \mathbb{Z}[\tau]$ such that $z = \alpha + \beta\zeta_5$ and, consequently, $z^{\star_5} = \alpha' + \beta'\zeta_5^3 \in W_\lambda$. By definition of W_λ, one has $z^{\star_5} = \Phi^\star(\mu)$, where $\mu \in H^{(\tau',0,1)}$ satisfies $\mu + (\lambda - t)^\star \in W$. Clearly, there exist $r, s \in \mathbb{R}$ such that $\mu = r(0,1,0)^t + s\frac{1}{2}(-1,-\tau,\tau')^t$, whence $\Phi^\star(\mu) = r + s\zeta_5^3$. The linear independence of 1 and ζ_5^3 over $\mathbb{R}$ now implies that $r = \alpha$ and $s = \beta$, so that $\mu \in L^\star$. Moreover, one can verify that one has $\mu^{-\star} \in (\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda$ and $\Phi(\mu^{-\star}) = \alpha + \beta\zeta_5 = z$. This proves the claimed identity. The assertion is now immediate. □

Example 3.17. For an illustration of the content of Proposition 3.16 in case of the icosahedral model set $\varLambda_{\mathrm{ico}}^{\mathrm{B}}$ from Example 3.7, see Figures 2 and 3.

3.3. **The translation module of icosahedral model sets.** In order to shed some light on the set of $\varLambda$-directions of an icosahedral model set $\varLambda$ with underlying $\mathbb{Z}$-module L, we first have to establish a relation between icosahedral model sets and their underlying $\mathbb{Z}$-modules. We denote by m_τ the $\mathbb{Z}[\tau]$-module endomorphism of $\mathbb{Q}(\tau)^3$, given by multiplication by τ, *i.e.*, $\alpha \mapsto \tau\alpha$. Furthermore, we denote by ${m_\tau}^\star$ the $\mathbb{Z}[\tau]$-module endomorphism of $(\mathbb{Q}(\tau)^3)^\star$, given by $\alpha^\star \mapsto (\tau\alpha)^\star$.

Lemma 3.18. *The map ${m_\tau}^\star$ is contractive with contraction constant $1/\tau \in (0,1)$,* i.e.*, the equality $\|{m_\tau}^\star(\alpha^\star)\| = (1/\tau)\,\|\alpha^\star\|$ holds for all $\alpha \in \mathbb{Q}(\tau)^3$.*

Proof. For $\alpha \in \mathbb{Q}(\tau)^3$, observe that $\|{m_\tau}^\star(\alpha^\star)\| = \|(\tau\alpha)^\star\| = \|\tau'\alpha^\star\| = (1/\tau)\,\|\alpha^\star\|$. □

Lemma 3.19. *Let $\varLambda$ be an icosahedral model set with underlying $\mathbb{Z}$-module L, say $\varLambda = \varLambda_{\mathrm{ico}}(t,W)$. Then, for any $F \in \mathcal{F}(L)$, there is an expansive homothety $h\colon \mathbb{R}^3 \to \mathbb{R}^3$ such that $h(F) \subset \varLambda$.*

Proof. From $\mathrm{int}(W) \neq \varnothing$ and the denseness of $L^\star$ in $\mathbb{R}^3$, one gets the existence of a suitable $\alpha_0 \in L$ with ${\alpha_0}^\star \in \mathrm{int}(W)$. Consider the open neighbourhood $V := \mathrm{int}(W) - {\alpha_0}^\star$ of 0 in

$\mathbb{R}^3$. Since the map $m_\tau{}^\star$ is contractive by Lemma 3.18 (in the sense which was made precise in that lemma), the existence of a suitable $k \in \mathbb{N}$ is implied such that $(m_\tau{}^\star)^k(F^\star) \subset V$. Hence, one has $\{(\tau^k\alpha + \alpha_0)^\star \mid \alpha \in F\} \subset \mathrm{int}(W) \subset W$ and, further, $h(F) \subset \varLambda$, where $h\colon \mathbb{R}^3 \to \mathbb{R}^3$ is the expansive homothety given by $x \mapsto \tau^k x + (\alpha_0 + t)$. □

As an easy application of Lemma 3.19, one obtains the following result on the set of $\varLambda$-directions for icosahedral model sets $\varLambda$.

Proposition 3.20. *Let $\varLambda$ be an icosahedral model set with underlying $\mathbb{Z}$-module L. Then, the set of $\varLambda$-directions is precisely the set of L-directions.*

Proof. Since one has $\varLambda - \varLambda \subset L$, every $\varLambda$-direction is an L-direction. For the converse, let $u \in \mathbb{S}^2$ be an L-direction, say parallel to $\alpha \in L \setminus \{0\}$. By Lemma 3.19, there is a homothety $h\colon \mathbb{R}^3 \to \mathbb{R}^3$ such that $h(\{0, \alpha\}) \subset \varLambda$. It follows that $h(\alpha) - h(0) \in (\varLambda - \varLambda) \setminus \{0\}$. Since $h(\alpha) - h(0)$ is parallel to α, the assertion follows. □

4. Complexity

In the practice of quantitative HRTEM, the determination of the rotational orientation of a quasicrystalline probe in an electron microscope can rather easily be achieved in the diffraction mode. This is due to the icosahedral symmetry of genuine icosahedral quasicrystals. However, the X-ray images taken in the high-resolution mode do not allow us to locate the examined sets. Therefore, as already pointed out in [4], in order to prove practically relevant and rigorous results, one has to deal with the *non-anchored case* of the whole *local indistinguishability class* (or LI-class, for short) $\mathrm{LI}(\varLambda)$ of a regular, generic icosahedral model set $\varLambda$, rather than dealing with the *anchored case* of a single fixed icosahedral model set $\varLambda$; recall Remark 3.6 for the equivalence relation given by local indistinguishability and compare also [18].

Remark 4.1. In the crystallographic case of a lattice L in $\mathbb{R}^3$, the LI-class of L consists of all translates of L in $\mathbb{R}^3$, *i.e.*, one has $\mathrm{LI}(L) = \{t+L \mid t \in \mathbb{R}^3\}$. In particular, $\mathrm{LI}(L)$ simply consists of one translation class. The entire LI-class $\mathrm{LI}(\varLambda_{\mathrm{ico}}(t, W))$ of a regular, generic icosahedral model set $\varLambda_{\mathrm{ico}}(t, W)$ can be shown to consist of all generic icosahedral model sets of the form $\varLambda_{\mathrm{ico}}(t, s + W)$ and all patterns obtained as limits of sequences of generic icosahedral model sets of the form $\varLambda_{\mathrm{ico}}(t, s + W)$ in the local topology (LT). Here, two patterns are ε-close if, after a translation by a distance of at most ε, they agree on a ball of radius $1/\varepsilon$ around the origin; see [3, 35]. Each such limit is then a subset of some $\varLambda_{\mathrm{ico}}(t, s + W)$, but s might not be in a generic position. Note that the LI-class $\mathrm{LI}(\varLambda)$ of an icosahedral model set $\varLambda$ contains *uncountably many* (more precisely, $2^{\aleph_0}$) translation classes; *cf.* [3] and references therein.

In view of the complication described above, we must make sure that we deal with finite subsets of *generic* icosahedral model sets of the form $\varLambda_{\mathrm{ico}}(t, s+W)$, *i.e.*, subsets whose $.^\star$-image lies in the *interior* of the window. This restriction to the generic case is the proper analogue of the restriction to *perfect* lattices and their translates in the crystallographic case. Analogous to the lattice case [15, 16] and the case of cyclotomic model sets [4], the main algorithmic problems of the discrete tomography of icosahedral model sets look as follows.

Definition 4.2 (Consistency, Reconstruction, and Uniqueness Problem)**.** Let $L = \mathrm{Im}(\mathbb{I})$ (resp., $L = \mathbb{I}_0$), let $W \subset \mathbb{R}^3$ be a window and let $u_1, \ldots, u_m \in \mathbb{S}^2$ be $m \geq 2$ pairwise non-parallel L-directions. The corresponding consistency, reconstruction and uniqueness problems are defined as follows.

> Consistency.
> Given functions $p_{u_j} : \mathcal{L}^3_{u_j} \to \mathbb{N}_0$, $j \in \{1, \ldots, m\}$, whose supports are finite and satisfy $\mathrm{supp}(p_{u_j}) \subset \mathcal{L}^L_{u_j}$, decide whether there is a finite set F which is contained in an element of $\mathcal{I}^{\mathrm{B}}_g(W)$ (resp., $\mathcal{I}^{\mathrm{F}}_g(W)$) and satisfies $X_{u_j}F = p_{u_j}$, $j \in \{1, \ldots, m\}$.
>
> Reconstruction.
> Given functions $p_{u_j} : \mathcal{L}^3_{u_j} \to \mathbb{N}_0$, $j \in \{1, \ldots, m\}$, whose supports are finite and satisfy $\mathrm{supp}(p_{u_j}) \subset \mathcal{L}^L_{u_j}$, decide whether there exists a finite subset F of an element of $\mathcal{I}^{\mathrm{B}}_g(W)$ (resp., $\mathcal{I}^{\mathrm{F}}_g(W)$) that satisfies $X_{u_j}F = p_{u_j}$, $j \in \{1, \ldots, m\}$, and, if so, construct one such F.
>
> Uniqueness.
> Given a finite subset F of an element of $\mathcal{I}^{\mathrm{B}}_g(W)$ (resp., $\mathcal{I}^{\mathrm{F}}_g(W)$), decide whether there is a different finite set F' that is also a subset of an element of $\mathcal{I}^{\mathrm{B}}_g(W)$ (resp., $\mathcal{I}^{\mathrm{F}}_g(W)$) and satisfies $X_{u_j}F = X_{u_j}F'$, $j \in \{1, \ldots, m\}$.

One has the following tractability result, which was proved for the case of B-type icosahedral model sets by combining the results from Section 3.2 with those presented in [4]; *cf.* [24, Theorem 3.33] for the details. The proof for the F-type case is similar and we prefer to omit the straightforward details here. Below, for $L \in \{\mathrm{Im}(\mathbb{I}), \mathbb{I}_0\}$, the L-directions in $\mathbb{S}^2 \cap H^{(\tau,0,1)}$ will be called *$L^{(\tau,0,1)}$-directions*. By Lemma 3.12(a), the set of $\mathrm{Im}(\mathbb{I})^{(\tau,0,1)}$-directions and the set of $\mathbb{I}_0^{(\tau,0,1)}$-directions coincide.

Theorem 4.3. *Let $L \in \{\mathrm{Im}(\mathbb{I}), \mathbb{I}_0\}$. When restricted to two $L^{(\tau,0,1)}$-directions and polyhedral windows, the problems* Consistency, Reconstruction *and* Uniqueness *as defined in Definition 4.2 can be solved in polynomial time in the real RAM-model of computation.*

Remark 4.4. For a detailed analysis of the complexities of the above algorithmic problems in the B-type case, we refer the reader to [24, Chapter 3]. Note that even in the anchored planar lattice case $\mathbb{Z}^2$ the corresponding problems Consistency, Reconstruction and Uniqueness are $\mathbb{NP}$-hard for three or more $\mathbb{Z}^2$-directions; *cf.* [15, 16].

5. Uniqueness

5.1. **Simple results on determination of finite subsets of icosahedral model sets.** In this section, we present some uniqueness results which only deal with the *anchored case* of determining finite subsets of a fixed icosahedral model set $\varLambda$ by X-rays in *arbitrary* $\varLambda$-directions; *cf.* Proposition 3.20. As already explained in Section 1, X-rays in non-$\varLambda$-directions are meaningless in practice. Without the restriction to $\varLambda$-directions, the finite subsets of a fixed icosahedral model set $\varLambda$ can be determined by one X-ray. In fact, any X-ray in a non-$\varLambda$-direction is suitable for this purpose, since any line in 3-space in a non-$\varLambda$-direction passes through at most one point of $\varLambda$. The next result represents a fundamental source of difficulties

in discrete tomography. There exist several versions; compare [21, Theorem 4.3.1], [13, Lemma 2.3.2], [5, Proposition 4.3], [24, Proposition 2.3 and Remark 2.4] and [23, Proposition 8].

Proposition 5.1. *Let $\varLambda$ be an icosahedral model set with underlying $\mathbb{Z}$-module L, say $\varLambda = \varLambda_{\text{ico}}(t, W)$. Further, let $U \subset \mathbb{S}^2$ be an arbitrary, but fixed finite set of pairwise non-parallel L-directions. Then, $\mathcal{F}(\varLambda)$ is not determined by the X-rays in the directions of U.*

Proof. We argue by induction on $\text{card}(U)$. The case $\text{card}(U) = 0$ means $U = \varnothing$ and is obvious. Suppose the assertion to be true whenever $\text{card}(U) = k \in \mathbb{N}_0$ and let $\text{card}(U) = k + 1$. By induction hypothesis, there are different elements F and F' of $\mathcal{F}(\varLambda)$ with the same X-rays in the directions of U', where $U' \subset U$ satisfies $\text{card}(U') = k$. Let u be the remaining direction of U. Choose a non-zero element $\alpha \in L$ parallel to u such that $\alpha + (F \cup F')$ and $F \cup F'$ are disjoint. Then, $F'' := (F \cup (\alpha + F')) - t$ and $F''' := (F' \cup (\alpha + F)) - t$ are different elements of $\mathcal{F}(L)$ with the same X-rays in the directions of U. By Lemma 3.19, there is a homothety $h\colon \mathbb{R}^3 \to \mathbb{R}^3$ such that $h(F'' \cup F''') = h(F'') \cup h(F''') \subset \varLambda$. It follows that $h(F'')$ and $h(F''')$ are different elements of $\mathcal{F}(\varLambda)$ with the same X-rays in the directions of U; *cf.* Lemma 2.6. □

Remark 5.2. An analysis of the proof of Proposition 5.1 shows that, for any finite set $U \subset \mathbb{S}^2$ of k pairwise non-parallel L-directions, there are disjoint elements F and F' of $\mathcal{F}(\varLambda)$ with $\text{card}(F) = \text{card}(F') = 2^{(k-1)}$ and with the same X-rays in the directions of U. Consider any convex subset C of $\mathbb{R}^3$ which contains F and F' from above. Then, the subsets $F_1 := (C \cap \varLambda) \setminus F$ and $F_2 := (C \cap \varLambda) \setminus F'$ of $\mathcal{F}(\varLambda)$ also have the same X-rays in the directions of U. Whereas the points in F and F' are widely dispersed over a region, those in F_1 and F_2 are contiguous in a way similar to atoms in a quasicrystal; compare [15, Remark 4.3.2] and [23, Remark 2.4 and Figure 2.1] (see also [23, Remark 32 and Figure 5]).

Originally, the proof of the following result is due to Rényi; *cf.* [32] and compare [21, Theorem 4.3.3].

Proposition 5.3. *Let $\varLambda$ be an icosahedral model set with underlying $\mathbb{Z}$-module L. Further, let $U \subset \mathbb{S}^2$ be any set of $k + 1$ pairwise non-parallel L-directions, where $k \in \mathbb{N}_0$. Then, $\mathcal{F}_{\leq k}(\varLambda)$ is determined by the X-rays in the directions of U. Moreover, for all $F \in \mathcal{F}_{\leq k}(\varLambda)$, one has $G_U^F = F$.*

Proof. Let $F, F' \in \mathcal{F}_{\leq k}(\varLambda)$ have the same X-rays in the directions of U. Then, one has $\text{card}(F) = \text{card}(F')$ by Lemma 2.2(a) and $F, F' \subset G_F^U$ by Lemma 2.4. But we have $G_F^U = F$ since the existence of a point in $G_F^U \setminus F$ implies the existence of at least $\text{card}(U) \geq k+1$ points in F, a contradiction. It follows that $F = F'$. □

Remark 5.4. In particular, the additional statement of Proposition 5.3 demonstrates that, for a fixed icosahedral model set $\varLambda$ with underlying $\mathbb{Z}$-module L, the unique reconstruction of sets $F \in \mathcal{F}_{\leq k}(\varLambda)$ from their X-rays in arbitrary sets of $k+1$ pairwise non-parallel L-directions $U \subset \mathbb{S}^2$ merely amounts to compute the grids G_F^U. Let $\varLambda$ be an icosahedral model set with underlying $\mathbb{Z}$-module L. Remark 5.2 and Proposition 5.3 show that $\mathcal{F}_{\leq k}(\varLambda)$ can be determined by the X-rays in any set of $k + 1$ pairwise non-parallel L-directions but not by $1 + \lfloor \log_2 k \rfloor$ pairwise non-parallel X-rays in L-directions. However, in practice, one is interested in the determination of finite sets by X-rays in a small number of directions since after about 3 to 5 images taken by HRTEM, the object may be damaged or even destroyed by the radiation

energy. Observing that the typical atomic structures to be determined comprise about 10^6 to 10^9 atoms, one realizes that the last result is not practical at all.

The following result was proved in [24, Theorem 2.8(a)]; see also [23, Theorem 13(a)].

Proposition 5.5. *Let $d \geq 2$, let $R > 0$, and let $\varLambda \subset \mathbb{R}^d$ be a Delone set of finite local complexity. Then, the set $\mathcal{D}_{<R}(\varLambda)$ is determined by two X-rays in $\varLambda$-directions.*

Since icosahedral model sets $\varLambda \subset \mathbb{R}^3$ are Delone sets of finite local complexity (*cf.* Remark 3.6), the following corollary follows immediately from Proposition 5.5 in conjunction with Proposition 3.20.

Corollary 5.6. *Let $\varLambda$ be an icosahedral model set with underlying $\mathbb{Z}$-module L and let $R > 0$. Then, the set $\mathcal{D}_{<R}(\varLambda)$ is determined by two X-rays in L-directions.*

Remark 5.7. Although looking promising at first sight, Corollary 5.6 is of limited use in practice because, in general, one cannot guarantee that all the directions which are used yield densely occupied lines in icosahedral model sets.

5.2. **Determination of convex subsets of icosahedral model sets.**

Remark 5.8. Proposition 3.20 shows that, for all icosahedral model sets $\varLambda$ with underlying $\mathbb{Z}$-module L, the set of $L^{(\tau,0,1)}$-directions is precisely the set of $\varLambda$-directions in $\mathbb{S}^2 \cap H^{(\tau,0,1)}$. Further, by Lemmas 3.14 and 3.15, the set of $L^{(\tau,0,1)}$-directions maps under Φ bijectively onto the set of $\mathbb{Z}[\zeta_5]$-directions.

The following property is evident.

Lemma 5.9. *Let $L \in \{\mathrm{Im}(\mathbb{I}), \mathbb{I}_0\}$, let $U \subset \mathbb{S}^2$ be a finite set of $L^{(\tau,0,1)}$-directions, and let $F, F' \in \mathcal{F}(t + H^{(\tau,0,1)})$, where $t \in \mathbb{R}^3$. If F and F' have the same X-rays in the directions of U, then $\Phi(F - t)$ and $\Phi(F' - t)$ have the same X-rays in the directions of $\Phi(U) \subset \mathbb{S}^1$.*

The following fundamental result follows immediately from [24, Theorem 2.54]; see also [23, Theorem 15].

Theorem 5.10. *The following assertions hold:*

(a) *There is a set $U \subset \mathbb{S}^1$ of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions such that, for all cyclotomic model sets $\varLambda_{\mathrm{cyc}}$ with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$, the set $\mathcal{C}(\varLambda_{\mathrm{cyc}})$ is determined by the X-rays in the directions of U.*

(b) *For all cyclotomic model sets $\varLambda_{\mathrm{cyc}}$ with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$ and all sets $U \subset \mathbb{S}^1$ of three or less pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions, the set $\mathcal{C}(\varLambda_{\mathrm{cyc}})$ is not determined by the X-rays in the directions of U.*

We are now able to prove the main result of this text by applying the results of [24, 23] on the determination of convex subsets of cyclotomic model sets with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$ to the various images $\Phi((\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$, where $\varLambda$ is an icosahedral model set and $\lambda \in \varLambda$.

Remark 5.11. Note that, for a convex subset C of an icosahedral model set $\varLambda$ and an element $\lambda \in \varLambda$, the intersection $C \cap (\lambda + H^{(\tau,0,1)})$ is a convex subset of the slice $\varLambda \cap (\lambda + H^{(\tau,0,1)})$ of $\varLambda$. Hence, $\Phi((C \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ is a convex subset of $\Phi((\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$.

The following fundamental result deals with the anchored case.

Theorem 5.12. *Let $L \in \{\mathrm{Im}(\mathbb{I}), \mathbb{I}_0\}$. The following assertions hold:*

(a) *There is a set $U \subset \mathbb{S}^2$ of four $L^{(\tau,0,1)}$-directions such that, for all generic icosahedral model sets $\varLambda$ with underlying $\mathbb{Z}$-module L, the set $\mathcal{C}(\varLambda)$ is determined by the X-rays in the directions of U.*

(b) *For all generic icosahedral model sets $\varLambda$ with underlying $\mathbb{Z}$-module L and all sets $U \subset \mathbb{S}^2$ of three or less pairwise non-parallel $L^{(\tau,0,1)}$-directions, the set $\mathcal{C}(\varLambda)$ is not determined by the X-rays in the directions of U.*

Proof. For part (a), let $U' \subset \mathbb{S}^1$ be a set of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions with the property that, for all cyclotomic model sets $\varLambda_{\mathrm{cyc}}$ with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$, the set $\mathcal{C}(\varLambda_{\mathrm{cyc}})$ is determined by the X-rays in the directions of U'. Such a set U' exists by Theorem 5.10(a). We claim that, for all generic icosahedral model sets $\varLambda$ with underlying $\mathbb{Z}$-module L, the set $\mathcal{C}(\varLambda)$ is determined by the X-rays in the directions of $U := \Phi^{-1}(U') \subset \mathbb{S}^2$. *Cf.* Remark 5.8 for the fact that U consists only of $L^{(\tau,0,1)}$-directions. Assume the existence of two different elements, say C and C', of $\mathcal{C}(\varLambda)$ having the same X-rays in the directions of U. Hence, there is an element $\lambda \in \varLambda$ such that $C \cap (\lambda + H^{(\tau,0,1)})$ and $C' \cap (\lambda + H^{(\tau,0,1)})$ are different convex subsets of the slice $\varLambda \cap (\lambda + H^{(\tau,0,1)})$ with the same X-rays in the directions of U. By Lemma 5.9 and Remark 5.11, it follows that $\Phi((C \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ and $\Phi((C \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ are different convex subsets of $\Phi((\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ having the same X-rays in the $\mathbb{Z}[\zeta_5]$-directions of U'. Since the set $\Phi((\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ is a cyclotomic model set with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$ by Proposition 3.16, this is a contradiction.

For assertion (b), let $U \subset \mathbb{S}^2$ be a set of three or less pairwise non-parallel $L^{(\tau,0,1)}$-directions and let $\varLambda$ be a generic icosahedral model set with underlying $\mathbb{Z}$-module L. Consider a slice $\varLambda \cap (\lambda + H^{(\tau,0,1)})$ of $\varLambda$, $\lambda \in \varLambda$, together with the cyclotomic model set $\Phi((\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$; *cf.* Proposition 3.16. By Theorem 5.10(b), there are two different convex subsets, say C and C', of $\Phi((\varLambda \cap (\lambda + H^{(\tau,0,1)})) - \lambda)$ with the same X-rays in the $\mathbb{Z}[\zeta_5]$-directions of $U' := \Phi(U) \subset \mathbb{S}^1$; *cf.* Remark 5.8. It follows that $\Phi^{-1}(C) + \lambda$ and $\Phi^{-1}(C') + \lambda$ are different convex subsets of (the slice $\varLambda \cap (\lambda + H^{(\tau,0,1)})$ of) $\varLambda$ with the same X-rays in the $L^{(\tau,0,1)}$-directions of U. □

Remark 5.13. The proof of Theorem 5.12 shows that the result extends to the set of subsets C of generic icosahedral model sets $\varLambda$ that are only $H^{(\tau,0,1)}$-*convex*, the latter meaning that, for all $\lambda \in \varLambda$, the sets $C \cap (\lambda + H^{(\tau,0,1)})$ are convex subsets of the slices $\varLambda \cap (\lambda + H^{(\tau,0,1)})$.

Example 5.14. It was shown in [24, Theorem 2.56 and Example 2.57] (see also [23, Theorem 16 and Example 3]) that the convex subsets of cyclotomic model sets with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$ are determined by the X-rays in the $\mathbb{Z}[\zeta_5]$-directions of $U_5 := \{o/|o| \mid o \in O\} \subset \mathbb{S}^1$, where $O := \{(1+\tau)+\zeta_5,\ (\tau-1)+\zeta_5,\ -\tau+\zeta_5, 2\tau-\zeta_5\} \subset \mathbb{Z}[\zeta_5] \setminus \{0\}$. Consequently, as was shown in the proof of Theorem 5.12(a), the convex subsets of generic icosahedral model sets $\varLambda$ with underlying $\mathbb{Z}$-module L are determined by the X-rays in the $L^{(\tau,0,1)}$-directions of $U_{\mathrm{ico}} := \Phi^{-1}(U_5) \subset \mathbb{S}^2$.

Remark 5.15. Since, by the work of Pleasants [31], the $\mathbb{Z}[\zeta_5]$-directions of U_5 are well suited in order to yield dense lines in cyclotomic model sets with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$, it follows that the set of $L^{(\tau,0,1)}$-directions U_{ico} from Example 5.14 is well suited in order to yield dense

lines in the corresponding slices $\varLambda \cap (\lambda + H^{(\tau,0,1)})$, $\lambda \in \varLambda$, of generic icosahedral model sets $\varLambda$ with underlying $\mathbb{Z}$-module L. In fact, these directions even yield dense lines in icosahedral model sets $\varLambda$ as a whole; *cf.* [31]. In particular, neighbouring slices of the form $\varLambda\cap(\lambda+H^{(\tau,0,1)})$, $\lambda \in \varLambda$, are densely occupied and hence well separated. Consequently, neighbouring lines in any of the directions of U that meet at least one point of a fixed icosahedral model set $\varLambda$ are sufficiently separated. It follows that, in the practice of quantitative HRTEM, the resolution coming from the above directions is likely to be rather high, which makes Theorem 5.12 look promising.

Finally, we want to demonstrate that, in an approximative sense, part (a) of Theorem 5.12 even holds in the non-anchored case for regular generic icosahedral model sets. Before, we need a consequence of Weyl's theory of uniform distribution; *cf.* [40]. This analytical property of regular icosahedral model sets was analyzed in general in [34], [35] and [28]. We need the following variant which relates the centroids of images of certain finite subsets of a regular icosahedral model set $\varLambda$ under the star map to the centroid of its window.

Theorem 5.16. *Let $\varLambda$ be a regular icosahedral model set of the form $\varLambda = \varLambda_{\mathrm{ico}}(0, W)$. Then, for all $a \in \mathbb{R}^3$, one has the identity*

$$\lim_{R\to\infty} \frac{1}{\mathrm{card}(\varLambda \cap B_R(a))} \sum_{\alpha\in\varLambda\cap B_R(a)} \alpha^\star \;=\; \frac{1}{\mathrm{vol}(W)} \int_W y \,\mathrm{d}\lambda(y)\,,$$

where λ denotes the Lebesgue measure on $\mathbb{R}^3$.

Proof. This is a consequence of the uniform distribution of the points of $\varLambda^*$ in the window, which gives the integral by Weyl's lemma. The proof of the uniform distribution property for model sets can be found in [34, 27, 28]. □

The following properties of sets $U \subset \mathbb{S}^1$ consisting of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions will be of crucial importance:

(C) For all cyclotomic model sets $\varLambda_{\mathrm{cyc}}$ with underlying $\mathbb{Z}$-module $\mathbb{Z}[\zeta_5]$, the set $\mathcal{C}(\varLambda_{\mathrm{cyc}})$ is determined by the X-rays in the directions of U.

(E) U contains two directions of the form $o/|o|, o'/|o'|$, where $o, o' \in \mathbb{Z}[\zeta_5] \setminus \{0\}$ satisfy the relation

$$\alpha_o\beta_{o'} - \beta_o\alpha_{o'} \;\in\; \mathbb{Z}[\tau]^\times = \{\tau^s \mid s \in \mathbb{Z}\}\,,$$

where the elements $\alpha_o, \alpha_{o'}, \beta_o, \beta_{o,} \in \mathbb{Z}[\tau]$ are determined by $o = \alpha_o + \beta_o\zeta_5$ and $o' = \alpha_{o'} + \beta_{o'}\zeta_5$; *cf.* Remark 3.8.

Example 5.17. The set $U_5 \subset \mathbb{S}^1$ of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions as defined in Example 5.14 has property (C) by [24, Example 2.57] (see also [23, Example 3]). Additionally, one can easily see that U_5 also has property (E).

The significance of property (E) is expressed by the following result.

Proposition 5.18. *Let $U \subset \mathbb{S}^1$ be a set of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions with property* (E)*. Then, for all finite subsets F of $\mathbb{Z}[\zeta_5]$, one has the inclusion*

$$G_U^F \;\subset\; \mathbb{Z}[\zeta_5]\,.$$

Proof. This follows from [24, Theorem 1.130] (see also [23, Theorem 12]). □

We are now able to show that, in an approximative sense to be clarified below, for any fixed window $W \subset \mathbb{R}^3$ whose boundary $\mathrm{bd}(W)$ has Lebesgue measure 0 in $\mathbb{R}^3$, the set $\cup_{\varLambda\in\mathcal{I}_g^{\mathrm{B}}(W)}\mathcal{C}(\varLambda)$ (resp., $\cup_{\varLambda\in\mathcal{I}_g^{\mathrm{F}}(W)}\mathcal{C}(\varLambda)$) is determined by the X-rays in any set of $L^{(\tau,0,1)}$-directions, where $L = \mathrm{Im}(\mathbb{I})$ (resp., $L = \mathbb{I}_0$), of the form $U := \Phi^{-1}(U')$, where U' is a set of four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions with the properties (C) and (E). Since the arguments for the F-type case and the B-type case are similar, we present the details for the B-type case only. Let

$$F, F' \;\in \bigcup_{\varLambda\in\mathcal{I}_g^{\mathrm{B}}(W)} \mathcal{C}(\varLambda)\,,$$

say $F \in \mathcal{C}(\varLambda_{\mathrm{ico}}^{\mathrm{B}}(t, s+W))$ and $F' \in \mathcal{C}(\varLambda_{\mathrm{ico}}^{\mathrm{B}}(t', s'+W))$, where $t, t', s, s' \in \mathbb{R}^3$, and suppose that F and F' have the same X-rays in the directions of U. If $F = \varnothing$, then, by Lemma 2.2(a), one also gets $F' = \varnothing$. One may thus assume, without loss of generality, that F and F' are non-empty. Hence, there is an element $\lambda \in F$ such that $F\cap(\lambda+H^{(\tau,0,1)})$ and $F'\cap(\lambda+H^{(\tau,0,1)})$ are non-empty finite sets with the same X-rays in the directions of U. Then, by Lemma 5.9, the non-empty finite subset $\Phi((F\cap(\lambda+H^{(\tau,0,1)}))-\lambda)$ of $\mathbb{Z}[\zeta_5]$ (*cf.* Lemma 3.15) and the non-empty finite subset $\Phi((F'\cap(\lambda+H^{(\tau,0,1)}))-\lambda)$ of $\mathbb{C}$ have the same X-rays in the four pairwise non-parallel $\mathbb{Z}[\zeta_5]$-directions of $\Phi(U) = U'$. Then, by Lemma 2.4 and Proposition 5.18 in conjunction with property (E), one obtains

$$\Phi((F \cap (\lambda + H^{(\tau,0,1)})) - \lambda), \Phi((F' \cap (\lambda + H^{(\tau,0,1)})) - \lambda) \subset G_{U'}^{\Phi((F\cap(\lambda+H^{(\tau,0,1)}))-\lambda)} \subset \mathbb{Z}[\zeta_5]\,.$$

Thus, one gets

$$F \cap (\lambda + H^{(\tau,0,1)}), F' \cap (\lambda + H^{(\tau,0,1)}) \;\subset\; t + L\,. \tag{6}$$

Since $F' \cap (\lambda + H^{(\tau,0,1)}) \subset t' + L$, Relation (6) implies that $t+L$ meets $t'+L$, the latter being equivalent to the identity $t+L = t'+L$. Note also that the identity $t+L = t'+L$ is equivalent to the relation $t'-t \in L$. Clearly, one has

$$F - t \;\in\; \mathcal{C}(\varLambda_{\mathrm{ico}}^{\mathrm{B}}(0, s+W))\,.$$

Moreover, since the equality

$$\varLambda_{\mathrm{ico}}^{\mathrm{B}}(t'-t, s'+W) = \varLambda_{\mathrm{ico}}^{\mathrm{B}}(0, (s'+(t'-t)^\star)+W)$$

holds, one further obtains

$$F' - t \;\in\; \mathcal{C}(\varLambda_{\mathrm{ico}}^{\mathrm{B}}(t'-t, s'+W)) \;=\; \mathcal{C}(\varLambda_{\mathrm{ico}}^{\mathrm{B}}(0, (s'+(t'-t)^\star)+W))\,.$$

Clearly, $F-t$ and $F'-t$ again have the same X-rays in the directions of U. Hence, by Lemma 2.2(b), $F-t$ and $F'-t$ have the same centroid. Since the star map $.^\star$ is $\mathbb{Q}$-linear, it follows that the finite subsets $(F-t)^\star$ and $(F'-t)^\star$ of $\mathbb{R}^3$ also have the same centroid. Now, if one has

$$F - t \;=\; B_R(a) \;\cap\; \varLambda_{\mathrm{ico}}^{\mathrm{B}}(0, s+W)$$

and

$$F' - t \;=\; B_{R'}(a') \;\cap\; \varLambda_{\mathrm{ico}}^{\mathrm{B}}(0, (s'+(t'-t)^\star)+W)$$

for suitable $a, a' \in \mathbb{R}^3$ and large $R, R' > 0$ (which is rather natural in practice), then Theorem 5.16 allows us to write

$$
\begin{aligned}
\frac{1}{\mathrm{vol}(W)}\int_{s+W} y\,\mathrm{d}\lambda(y) \;&\approx\; \frac{1}{\mathrm{card}\,(F-t)}\sum_{x\in F-t} x^{\star}\\
&=\; \frac{1}{\mathrm{card}\,(F'-t)}\sum_{x\in F'-t} x^{\star}\\
&\approx\; \frac{1}{\mathrm{vol}(W)}\int_{(s'+(t'-t)^{\star})+W} y\,\mathrm{d}\lambda(y)\,.
\end{aligned}
$$

Consequently,

$$
s+\int_{W} y\,\mathrm{d}\lambda(y) \;\approx\; (s'+(t'-t)^{\star})+\int_{W} y\,\mathrm{d}\lambda(y)\,,
$$

and hence $s \approx s'+(t'-t)^{\star}$. The latter means that, approximately, both $F-t$ and $F'-t$ are elements of the set $\mathcal{C}(\varLambda_{\mathrm{ico}}^{\mathrm{B}}(0,s+W))$. Now, it follows in this approximative sense from property (C) and Theorem 5.12 that $F-t \approx F'-t$, and, finally, $F \approx F'$.

Remark 5.19. The above analysis suggests that, for all fixed windows $W \subset \mathbb{R}^3$ whose boundary $\mathrm{bd}(W)$ has Lebesgue measure 0 in $\mathbb{R}^3$, the sets of the form $\cup_{\varLambda\in\mathcal{I}_g^{\mathrm{B}}(W)}\mathcal{C}(\varLambda)$ (resp., $\cup_{\varLambda\in\mathcal{I}_g^{\mathrm{F}}(W)}\mathcal{C}(\varLambda)$) are approximately determined by the X-rays in the four prescribed $L^{(\tau,0,1)}$-directions of U_{ico}, where $L=\mathrm{Im}(\mathbb{I})$ (resp., $L=\mathbb{I}_0$); *cf.* Examples 6.12 and 6.15. Additionally, in the practice of quantitative HRTEM, the resolution coming from the directions of U_{ico} is likely to be rather high, which makes this approximative result look even more promising in view of real applications; *cf.* Remark 5.15.

6. Outlook

For a more extensive account of both uniqueness and computational complexity results in the discrete tomography of Delone sets with long-range order, we refer the reader to [24]. This reference also contains results on the interactive concept of *successive determination* of finite sets by X-rays and further extensions of settings and results that are beyond our scope here; compare also [23]. Although the results of this text and of [24] give satisfying answers to the basic problems of discrete tomography of icosahedral model sets, there is still a lot to do to create a tool that is as satisfactory for the application in materials science as is computerized tomography in its medical or other applications. First, we believe that it is an interesting problem to characterize the sets of $\varLambda$-directions *in general position* having the property that, for all icosahedral model sets $\varLambda$, the set of convex subsets of $\varLambda$ is determined by the X-rays in these directions; compare [13, Problems 2.1 and 2.3]. Secondly, it would be interesting to have experimental tests in order to see how well the above results work in practice. Since there is always some noise involved when physical measurements are taken, the latter also requires the ability to work with imprecise data. For this, it is necessary to study stability and instability results in the discrete tomography of icosahedral model sets in the future; *cf.* [1].

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